Cooper-pair transport through a Hubbard chain sandwiched between two superconductors: Density matrix renormalization group calculations

Adrian E. Feiguin
Microsoft Project Q
The University of California at Santa Barbara,
Santa Barbara, CA 93106[*]

Steven R. White
Department of Physics and Astronomy
University of California, Irvine, CA 92697[†]

D. J. Scalapino
Department of Physics
University of California, Santa Barbara, CA 93106-9530[‡]
(Dated: February 6, 2008)

We present a numerical approach to study the coherent transport of Cooper pairs through a Hubbard chain, and study the role of the contacts in achieving perfect Andreev reflection. We calculate the pair transport using the Density Matrix Renormalization Group by measuring the response of the system to quantum pair fields with complex phases on the two ends of an open system. This approach gives an effective superfluid weight which is in close agreement with the Bethe Ansatz results for the superfluid weight for closed Hubbard rings.

PACS numbers: 74.45.+c,74.50.+r,71.10.Pm,03.67.Mn

I. INTRODUCTION

Pair transport through interacting one-dimensional systems sandwiched between two superconductors has been the focus of much attention recently. These systems not only exhibit interesting physical phenomena, such as Andreev reflection and pair transport, but also may be incorporated into novel nanoelectronic devices. In particular, there have been various proposals for the creation and transport of entangled pairs for quantum communication. Therefore, it is useful to have well-controlled numerical tools for analyzing phenomena associated with pair transport through a superconducting-Hubbard-superconducting (SHS) system.

In this paper we present the results of numerical studies of a one-dimensional Hubbard chain sandwiched between two superconducting contacts. We examine the effects of the boundary contacts on the injection and transport of pairs through the system. We then introduce the idea of an extended contact between the superconductors and the intervening Hubbard chain which provides for improved pair transmission into and out of the Hubbard chain. Using this we present a new numerical method for determining the effective superfluid weight $\tilde{D}$ of a Hubbard chain.

II. THE CONTACT MODEL

There have been various analytic studies of a one-dimensional Luttinger liquid sandwiched between two superconductors[1,2,3]. Here, we make use of a comprehensive analysis recently reported by Affleck *et. al*[4]. These authors integrated out the electron degrees of freedom of the superconducting leads, replacing them with effective boundary conditions for the Luttinger liquid. In this framework, the effective Hamiltonian for an SHS system can be written as

$$H = H_0 + H_1 \tag{1}$$

where H_0 corresponds to the Hubbard chain

$$H_0 = -t \sum_{\substack{i=1 \\ \sigma}}^{L} \left(c^\dagger_{i\sigma} c_{i+1\sigma} + h.c. \right) + U \sum_{i=1}^{L} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i=1}^{L} n_i \tag{2}$$

and H_1 incorporates the effects of the two superconducting leads

$$\begin{aligned} H_1 \; &= \; \Delta_L \left(e^{i\phi_L} c^\dagger_{1\uparrow} c^\dagger_{1\downarrow} + h.c. \right) + \Delta_R \left(e^{i\phi_R} c^\dagger_{L\uparrow} c^\dagger_{L\downarrow} + h.c. \right) \\ &+ \; V_1 (n_{1\uparrow} + n_{1\downarrow}) + V_L (n_{L\uparrow} + n_{L\downarrow}) \,. \end{aligned} \tag{3}$$

Here, $c^\dagger_{\ell\uparrow}$ creates an electron of spin up on the $\ell^{\rm th}$ site. The hopping parameter of the Hubbard chain is t, U is the onsite interaction energy, and μ is the usual chemical potential. As discussed in reference[4], the effect of the two superconducting leads can be parametrized in terms of contact pairing strengths $\Delta_{(L,R)}$ and their phases $\phi_{(L,R)}$, along with end point scattering potentials V_1 and V_L.

In the following we will be interested in the symmetric case in which $\Delta_L = \Delta_R = \Delta$ and $V_1 = V_L = V$. The first term in H_1 injects or removes pairs with different phases on both ends. In addition, there are effective boundary scattering potentials $V_{(1,L)}$ which arise and play an important role in achieving optimal pair transmission across

the ends of the Hubbard chain. Integrating out the superconducting electron degrees-of-freedom can be seen as a natural thing to do when the Fermi level lies well below the superconducting gaps in the bulk of the superconductors, since the pair fields in the superconductors have well-defined average values and negligible fluctuations. In the Hubbard system, the value of the pair field has to be replaced by the fluctuating pair operator. A similar approach was used by Kozub[5] to study Josephson transport through a Hubbard impurity center.

In their paper, Affleck, *el. al*[4] calculate the Josephson current and the Andreev reflection probability. For the non-interacting half-filled tight-binding chain, they find that the maximum transmission probability is 1 (perfect Andreev reflection) and it occurs when $\Delta = t$ and $V = 0$. In this case, the Josephson current versus the phase difference $\phi = \phi_R - \phi_L$ between the ends has Ishii's sawtooth form[6]. For smaller values of V, the sawtooth is smoothed out and starts resembling the Josephson sine shape corresponding to a small Andreev reflection probability (See also, Ref.[7]). Away from half-filling, Affleck *et. al* found that in order to achieve perfect Andreev reflection, both the contact pairing strength Δ and the boundary scattering potential V needed to be tuned to particular values. For the non-interacting case, these values are:

$$V = \frac{\mu}{2};\ \Delta = t\sqrt{1 - \frac{\mu^2}{4t^2}}\,. \tag{4}$$

In order to treat the interacting case, these authors employed bosonization and renormalization group methods. For negative values of U, they showed that the contact Hamiltonian renormalizes to the perfect Andreev reflection fixed point. Thus, even when the parameters of the contact were not fine-tuned for perfect Andreev reflection, one recovers the sawtooth form for the Josephson current versus the phase difference as the length L of the Luttinger liquid increases. However, for positive U, they found that the contact Hamiltonian flows away from the Andreev fixed point. In this case, as L increases, the effective coupling of the superconductor to the Luttinger liquid renormalizes to zero. For a finite value of L and $U > 0$, the coupling is weak and one finds the usual $J_1 \sin\phi$ Josephson relation. As L increases, J_1 rapidly decreases and the transport of pairs through the chain vanishes in the $L \to \infty$ limit.

III. THE EFFECTIVE SUPERFLUID WEIGHT $\tilde{D}$

In the following numerical study, we will be interested in determining an effective superfluid weight $\tilde{D}$. If the pair phase varies linearly across a Hubbard chain of length L, then there will be a uniform Josephson current, and we will define $\tilde{D}(L)$ by

$$j = \tilde{D}\frac{\phi_0}{L} \tag{5}$$

with ϕ_0 the phase difference across the Hubbard chain. The effective superfluid weight $\tilde{D}$ is then given by $\tilde{D}(L)$ as $L \to \infty$. Here, we have set $e = \hbar = 1$. The problem of determining $\tilde{D}(L)$ is to create a linear phase change ϕ_0/L across the Hubbard chain and then to measure j. The latter is straightforward since

$$j_i = -i[H, n_i] \tag{6}$$

so that for $i \neq 1$ or L,

$$j_i = -it\sum_\sigma \left(c^\dagger_{i\sigma}c_{i+1\sigma} - c^\dagger_{i+1\sigma}c_{i\sigma}\right)\,. \tag{7}$$

At the boundary, when $i = 1$ (or L) we have to consider the boundary terms and add an extra current operator

$$j'_1 = -iV(\exp(i\phi)c^\dagger_{1\uparrow}c^\dagger_{1\downarrow} - \exp(-i\phi)c_{1\downarrow}c_{1\uparrow})\,. \tag{8}$$

with a similar term for the right hand $i = L$ boundary. The current density is independent of the position, and any of these expressions can be used with these end corrections to calculate j.

The measurement of j is straightforward within the DMRG method[9,10]. However, it is also necessary to establish a uniform phase gradient. As noted in the previous section, for a finite length L of the Hubbard chain, this can require tuning of the contact boundary pairing strength and the boundary scattering potential. Fortunately, for negative values of U, the contact interaction renormalizes to the perfect Andreev reflection fixed point as the length of the chain increases. However, when the finite system is doped away from half-filling, there are two parameters to tune and achieving a match such that the phase gradient over the length L is uniform becomes more difficult. For this reason, we have developed an approach based upon extended contact interaction which will be discussed at the end of the next section.

IV. RESULTS

We use the Lanczos method for a system of size $L = 8$ and DMRG for larger systems. The DMRG method is the standard finite-size algorithm, except for the use of complex numbers due to the arbitrary Josephson phases, and a special treatment of quantum numbers. The non-particle conserving boundary conditions mean that the total number of fermions cannot be used as a conserved quantum number. However, one can still utilize the number of fermions modulo 2. This modulo-2 approach was first used in[11]. Within this approach the local pair-field Δ can take on a definite nonzero value. We have typically kept $m = 200$ states per block for the results presented, with a truncation error of about 10^{-8}.

A. Point Contacts

In Fig.1 we show Lanczos results for the Josephson current versus $\phi = \phi_R - \phi_L$ through a half-filled Hubbard

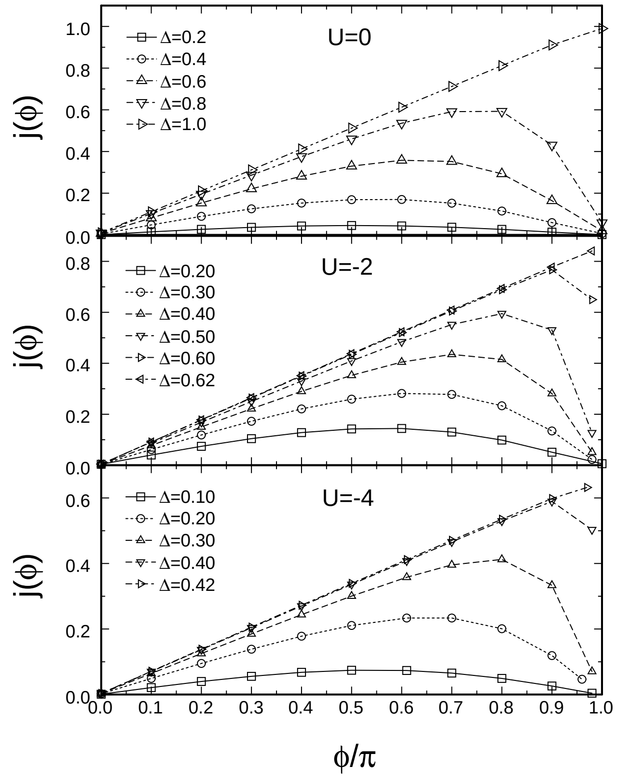

FIG. 1: Josephson current though a half-filled Hubbard chain with $L = 8$ as a function of the phase ϕ and for different values of the contact pairing Δ, and Coulomb interaction U, in units where the hopping $t = 1$.

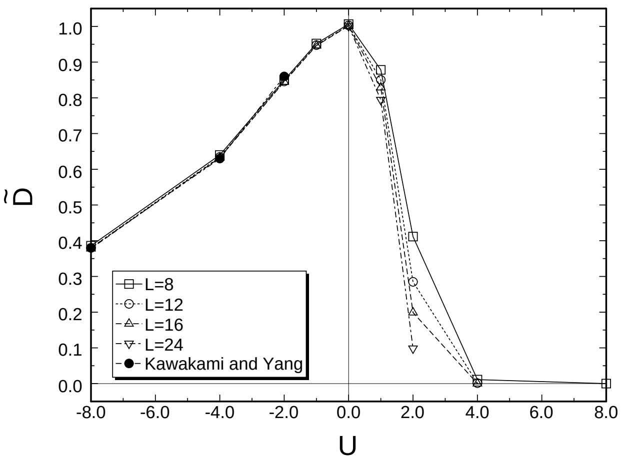

FIG. 2: Effective superfluid weight $\tilde{D}(L)$ of the half-filled Hubbard chain as a function of the Coulomb interaction U, for $\Delta = 1$, $V = 0$, and chains of various lengths. We add for comparison the exact $L \to \infty$ Bethe Ansatz results from[8] for $U < 0$.

chain of $L = 8$ sites. For this half-filled, particle-hole symmetric case, with $U \leq 0$, the required site potential $V_{1,L} = 0$ and the contact pairing strength Δ can be adjusted to achieve perfect Andreev reflection. For the non-interacting case, this is obtained for $\Delta/t = 1$ as shown in the top panel of Fig.1. For negative values of U, it is necessary to fine-tune Δ. When perfect Andreev reflection is achieved, $j_1(\phi)$ exhibits a sawtooth form with $j(\phi) = \tilde{D}(L)\phi/L$ for $-\pi \leq \phi \leq \pi$. In this case, $\tilde{D}(L)$ can be directly determined from $j(\phi)$. For negative values of U, $\tilde{D}$ rapidly approaches its asymptotic value when $L \gg \pi t/|U|$, so that the important requirement for determining $\tilde{D}$ is to achieve perfect Andreev reflection at the ends.

In Figure 2, we show Lanczos and DMRG results for the superfluid weight $\tilde{D}(L)$ of the half-filled chain for different values of the Coulomb interaction U. Here we have set $V = 0$ and taken $\Delta = 1$. The renormalization to perfect Andreev reflection is rapid for $U < 0$ and the resulting effective superfluid weight $\tilde{D}(L)$ varies little with L giving a value in close agreement with the exact Bethe-Ansatz results for the superfluid weight of the infinite system, taken from[8]. For $U > 0$, the system renormalizes as L increases to the non-superconducting fixed point and the Josephson current is rapidly suppressed.

In Fig.3 we show the DMRG results for the pair field amplitude along a chain at half-filling. The phase clearly varies linearly for negative U, while for positive values the modulus decays in a very short distance, a signature of the absence of superconductivity, and the phase order is disrupted by the small amount of noise in the DMRG.

For the 8-site chain, we have seen that for the half-filled, particle-hole symmetric case it is necessary to tune the contact pairing strength Δ in order to achieve perfect Andreev reflection. For the non half-filled case, for finite L, there are two contact coupling parameters, Δ and V, that require tuning.

In Fig.4 we show DMRG results for the superfluid weight versus electron density and various values of the Coulomb interaction. Here, n is the electron density in the bulk of the chain, *i.e.* the center of the chain and far from the contacts). For comparison we show results for the superfluid weight D_s for $L \to \infty$ obtained from Bethe Ansatz calculations[8]. For $U = 0$ we have adjusted the values of Δ and V for maximum transmitivity, Eq. 4. For finite U we have set $\Delta = 1$ and $V_{1,L} = 0$, *i.e.* they are not *optimized for perfect reflection*.

In Fig.5 we show plots of $\tilde{D}$ versus n for $U = -2$ and chains of different lengths L. As L increases, $\tilde{D}$ approaches the exact result as the point contact boundary condition renormalizes to perfect Andreev reflection. However, to control this convergence it is in principle necessary to extrapolate the result to zero DMRG truncation error (large number of states m) and then take the infinite length limit[12]. Hence, we would expect these curves to be more accurate if we were to fine-tune the parameters. However, this task has proven to be difficult. In order to overcome the difficulties of fine tuning the parameters in the Hamiltonian for optimal transmitance, we have stud-

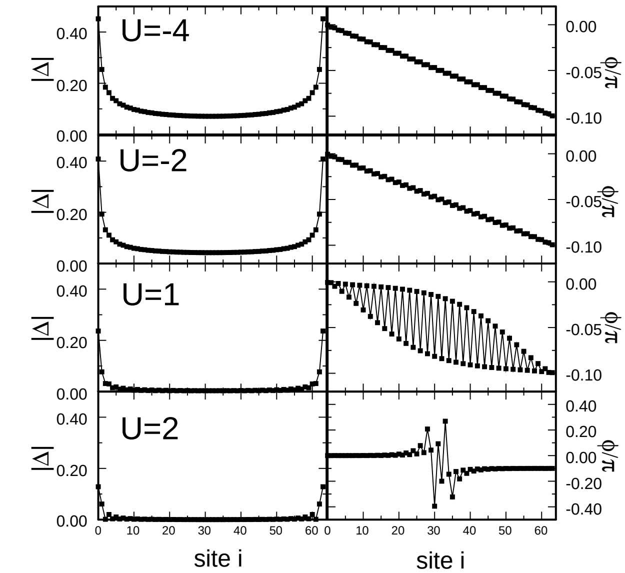

FIG. 3: Pair field amplitude and phase along the $L = 64$ chain for different values of U at half-filling.

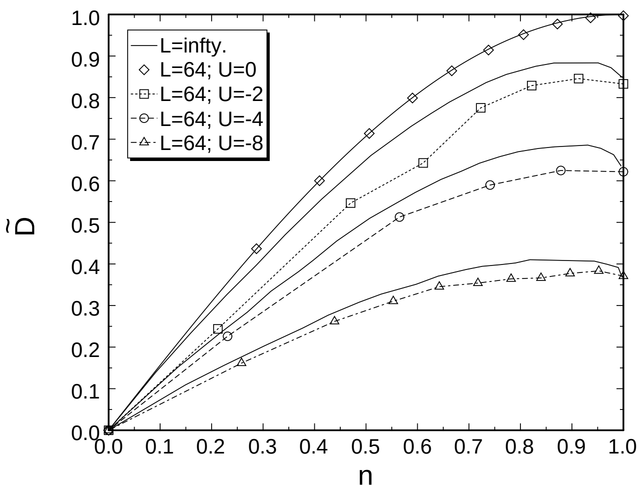

FIG. 4: $\tilde{D}$ as a function of the electron density for different values of the Coulomb interaction U. For $U = 0$, the boundary fields have been adjusted using Eqs.(4) to achieve perfect Andreev reflection, while for $U < 0$ we used $\Delta = 1$, and $V_{1,L} = 0$. We add for comparison the exact Bethe-Ansatz results from[8] (solid lines).

ied the effects of using extended smooth contacts at the boundaries.

B. Extended contacts

In the previous section we have discussed a Hubbard chain of finite length L connected to superconductors through point contacts. We have seen that it is necessary to tune the pairing strength Δ and the boundary scattering potential V in order to obtain a linear phase change along the chain. In this section, we explore the effects of extended contacts as an alternative way to eliminate the normal contact reflection. This technique is inspired by the smooth boundary conditions approach[13]. Here, we have applied the pair field end terms over a length ℓ_c on the end of each chain, with the coefficient dropping smoothly to zero as the distance from the end approaches ℓ_c. We have

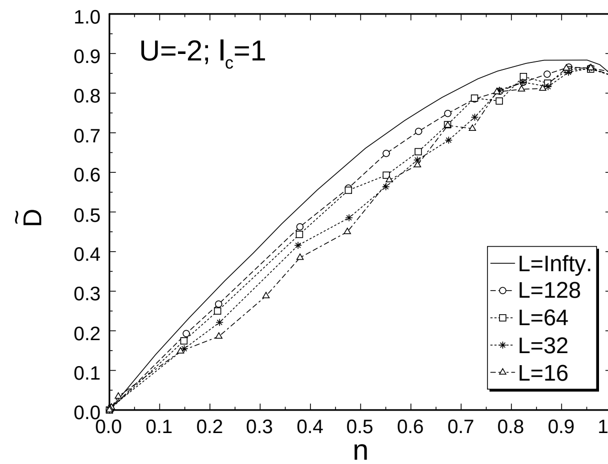

FIG. 5: Effective superfluid weigth $\tilde{D}$ of a Hubbard chain with $U = -2$, connected to point contacts, as a function of density n, and for different lengths L. We add for comparison the Bethe Ansatz results in the thermodynamic limit (solid line).

$$
\begin{aligned}
H_1 \;=\; & \sum_{\ell=1}^{\ell_c} \Delta(\ell)\left(e^{i\phi_L} c^\dagger_{\ell\uparrow} c^\dagger_{\ell\downarrow} + h.c.\right) \\
& + \sum_{\ell=L-\ell_{c+1}}^{L} \Delta(L-\ell)\left(e^{i\phi_R} c^\dagger_{\ell\uparrow} c^\dagger_{\ell\downarrow} + h.c.\right) \\
& + \sum_{\ell=1}^{\ell_c} V(\ell) n_\ell + \sum_{\ell=L-\ell_c+1}^{L} V(L-\ell+1) n_\ell \qquad (9)
\end{aligned}
$$

where we take $\Delta(x) = \Delta(1+\cos(x\pi/\ell_c))/2$[14]. In the following, we will set $V(x) = 0$ and examine various widths ℓ_c of the contact.

In calculating the superfluid weight with the extended contacts one must utilize only the local properties in the center of the system. In particular, one must measure the current and the gradient of the phase in the center of the system. The phase varies linearly in the central region of the chain, and this allows a numerical calculation of its gradient. It can also be shown that the effective superfluid weight can be extracted from the quantity[1]:

$$J = \int_0^L j(x)dx = \tilde{D}(L)\phi. \qquad (10)$$

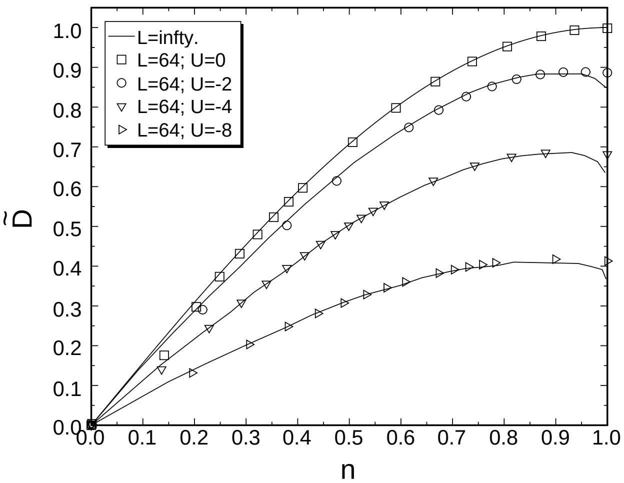

FIG. 6: Effective superfluid weight of a Hubbard chain ($L = 64$) connected to smooth contacts of width $\ell_c = 20$, as a function of density n, and for different values of U. We add for comparison the Bethe Ansatz results in the thermodynamic limit (solid lines).

In our calculations we simply replaced the integral by a sum over all the links. We find that the results obtained using the two approaches agree to within 1%.

Figure 6 shows the results for the effective superfluid weight $\tilde{D}$ for a Hubbard chain of length $L = 64$ with contacts of width $\ell_c = 20$. As in Fig.4, the solid lines are the Bethe-Ansatz results for D_s in the thermodynamic limit. As one can see, the DMRG results are in close agreement with the Bethe-ansatz results, except for $n = 1$. It may be that logarithmic contributions affect the convergence of the DMRG for $n = 1$[8]. The extended contact approach provides a much closer match between the supeconducting leads and the Hubbard chain so that we have essentially achieved perfect Andreev boundary conditions without any need for tuning of parameters.

V. CONCLUSIONS

Here we have reported results of a numerical study of a one-dimensional Hubbard model coupled to external pair fields. DMRG calculations typically use open boundary conditions making it simple to couple the ends of an interacting system to a classical potential or magnetic fields. Here we have explored the numerics involved in coupling to a quantum pair field which can inject or remove pairs of electrons. We have seen how the pair transport varies as a function of the interaction U, the filling $\langle n\rangle$ and the length of the Hubbard chain. Various current-phase relations associated with the degree of Andreev reflection were clearly seen. A phenomenological effective superfluid weight $\tilde{D}$ was introduced and found to be in close agreement with Bethe-ansatz results for the superfluid weight of an infinite ring.

Finally, the idea of an extended pair transfer contact was introduced. This was found to provide a useful way to effectively match the pair field injection such that the Andreev reflection approached unity. This is reminiscent of the extended tapered connections used to match waveguides with different propagation characteristics and may prove useful in obtaining optimal matching of bulk leads to nanowires.

Acknowledgments

SRW acknowledges the support of the NSF under grant DMR03-11843, and DJS acknowledges support from the Center of Nanophase Material Science at Oak Ridge National Laboratory (Tennessee). We would like to thank Ian Affleck for insightful discussions.

[*] Electronic address: afeiguin@microsoft.com
[†] Electronic address: srwhite@uci.edu
[‡] Electronic address: djs@vulcan2.physics.ucsb.edu

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[14] Asymptotically, as $\ell_c \to \infty$, one would expect a smoothing function with all derivatives continuous to be superior to this function which has a discontinuity in the second derivative. However, for small to moderate ℓ_c this function gives excellent results.